A DISCRIMINANT APPROACH TO PARAMETER ESTIMATION IN THE LINEAR MODEL WITH UNKNOWN VARIANCE–COVARIANCE MATRIX

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ABSTRACT

An estimate of the nonrandom vector, β, of parameters is obtained in the linear model $Y = X\beta + \varepsilon$, where ε is an unobservable random vector of disturbances and is assumed to satisfy $E(\varepsilon) = 0$ (the zero vector) and $E(\varepsilon\varepsilon^T) = V$, with V assumed unknown. The estimate obtained is the one which yields maximal similarity to the sample $Y_1, Y_2, \cdots, Y_N$ via the Sebestyen similarity function. Under the normality assumption, the resulting estimate is seen to be an unbiased estimate and justification given for selecting the maximum likelihood estimate for V in the Gauss-Markov estimate for B.

1. INTRODUCTION

Consider the linear model $Y = X\beta + \varepsilon$, where Y is an $n \times 1$ observable random vector, X is an $n \times m$ matrix of fixed elements and $\text{rank}(X) = m \leq n$, β is an $m \times 1$ nonrandom vector of parameters to be estimated and ε is an unobservable random vector of disturbances with ε assumed to satisfy $E(\varepsilon) = 0$ with unknown variance-covariance matrix $E(\varepsilon\varepsilon^T) = V$. It is well known that in case V is known (up to at least a scalar multiple), the Gauss-Markov theorem [1] applies and the best linear unbiased estimate of β is given by

$$\hat{\beta} = \left(X^T V^{-1} X\right)^{-1} X^T V^{-1} Y \qquad (1)$$

Other authors [2, 3, 4] have considered the problem of obtaining optimal estimates for β when V is unknown. Rao [4] showed that the estimate of β obtained by merely substituting an estimate $\hat{V}$ for V in equation (1) is not necessarily best; in particular, it may be possible to use known or inferred knowledge of the covariance V to obtain an estimator with better characteristics. Born [2] has written a recursive estimator when V is not known but is assumed to be block diagonal with equal diagonal blocks. McElroy [3] obtained necessary and sufficient conditions on V for equation (1) to be equivalent to the least-squares solution

$$\hat{\beta} = \left(X^T X\right)^{-1} X^T Y \qquad (2)$$

In this paper, we assume that the only available information is that contained in a sample $Y_1, Y_2, \cdots, Y_N$, and an estimate, $\hat{\beta}$, of β is obtained which results in maximal similarity to the given sample via the Sebestyen [5] similarity function. The resulting estimate appears in the form of equation (1), with V replaced by the standard (and in the normal theory case, the maximum likelihood) estimate of the variance-covariance matrix.

2. THE SEBESTYEN INTERSET SIMILARITY FUNCTION

If R^n denotes Euclidean n-space and P is the class of finite sequences of sample observations in R^n (i.e., $W, Z \in P$, provided $W = \{W_1, W_2, \cdots, W_N\}$ and $Z = \{Z_1, Z_2, \cdots, Z_M\}$ where $W_i, Z_j \in R^n$ for $i = 1, 2, \cdots, N$; $j = 1, 2, \cdots, M$), the Sebestyen [5] similarity function is defined as follows.

Definition: If $W, Z \in P$ with N and M elements, respectively, and if A is any $m \times n$ matrix, define the function $S_A: P \times P \to R_0$, where R_0 is the set of nonnegative real numbers, by

$$S_A(W,Z) = \frac{1}{NM} \sum_{i=1}^{N} \sum_{j=1}^{M} (W_i - Z_j)^T A^T A (W_i - Z_j) \qquad (3)$$

(The superscript T denotes the transpose.) Given a transformation A, $S_A(W,Z)$ is a measure of the similarity of the two samples W and Z in the transformed space (i.e., the resulting space after transforming R^n by A), and if W and Z are random samples from populations π_1 and π_2, respectively, then $S_A(W,Z)$ may be considered as a measure of the similarity of π_1 to π_2.

If $W,Z \in P$ have sample variance-covariance matrices $\hat{V}_1$ and $\hat{V}_2$, respectively, that is,

$$\left.\begin{aligned} \hat{V}_1 &= \frac{1}{N} \sum_{i=1}^{N} (W_i - \overline{W})(W_i - \overline{W})^T \\ \hat{V}_2 &= \frac{1}{M} \sum_{i=1}^{M} (Z_i - \overline{Z})(Z_i - \overline{Z})^T \end{aligned}\right\} \qquad (4)$$

and Tr denotes the trace operator [and $S(W,Z) \triangleq S_I(W,Z)$], then the properties below are easily verified.

Properties:

1. $S_A(W,Z) = \mathrm{Tr}\left[A(\hat{V}_1 + \hat{V}_2)A^T\right] + (\overline{W} - \overline{Z})^T A^T A (\overline{W} - \overline{Z})$.
2. $S(W,W) = 2\mathrm{Tr}(\hat{V}_1)$ and $S_A(W,W) = 2\mathrm{Tr}\left(A\hat{V}_1 A^T\right)$.
3. $S_A(W,Z) = S_A(Z,W)$.
4. $S_A(W,Z) \geq 0$ for every $W,Z \in P$ and for each $m \times n$ matrix.
5. If $V \in R^n$ then $S_A(W,V) = S_A(W,\{V\}) = \mathrm{Tr}\left(A\hat{V}_1 A^T\right)$ $+ (\overline{W} - V)^T A^T A (\overline{W} - V)$.
6. If $W = \{W_1, W_2, \cdots, W_N\}$ and $Z = \{Z_1, Z_2, \cdots, Z_M\}$, then $\frac{1}{M} \sum_{j=1}^{M} S_A(W,\{Z_j\}) = S_A(W,Z)$.

The Sebestyen decision rule is to classify an unknown u as belonging to category W provided

$$S_A(W,\{u\}) < S_B(Z,\{u\}) \tag{5}$$

where A and B are preselected transformations for W and Z, respectively. Consequently, the function $f(u) = S_B(Z,\{u\}) - S_A(W,\{u\})$ is the discriminant function for the Sebestyen decision rule, with classification of u into W or Z being accomplished by noting the sign of f(u); that is, u is classified as belonging to W or Z depending on whether $f(u) > 0$ or $f(u) < 0$, respectively.

3. A TRANSFORMATION TO MINIMIZE THE INTRASET DISTANCE

Thus far, no specifications have been placed on the transformation A; however, if A is an orthogonal matrix, the transformation results in a rotation of the original space whereby distances and, hence, angles are preserved. If the determinant of A [Det(A)] is 1, A is a volume-preserving transformation. The transformation of interest in this paper is specified in Theorem 1, the proof of which is dependent on the following well-known relationship between the arithmetic and geometric mean.

Lemma 1: If $d_i \geq 0$ for $i = 1, 2, \cdots, n$, then

$$\frac{1}{n}\sum_{i=1}^{n} d_i \geq \left(\prod_{i=1}^{n} d_i\right)^{1/n} \tag{6}$$

with equality holding if and only if $d_1 = d_2 = \cdots = d_n$.

Theorem 1: Under the condition Det(A) = 1 and S_A is positive definite, an $n \times n$ matrix A minimizes $S_A(W,W)$ [that is, the

similarity of a set with itself] if and only if $A\hat{V}_1A^T = \lambda I$, where $\lambda = [\mathrm{Det}(\hat{V}_1)]^{1/n}$ and $\hat{V}_1$ is the sample variance-covariance matrix of W specified in equation (4).

Proof: If B is any n × n matrix with Det(B) = 1 and A is the matrix specified in the hypothesis, from Property 3 and the fact that $A\hat{V}_1A^T = \lambda I$, we have $S_B(W,W) - S_A(W,W) = 2\mathrm{Tr}\left(B\hat{V}_1B^T\right) - 2n\lambda$. Letting U be the orthogonal matrix such that $UB\hat{V}_1B^TU^T = D$, where D is diagonal, then

$$\begin{aligned} 2\mathrm{Tr}\left(B\hat{V}_1B^T\right) - 2n\lambda &= 2\mathrm{Tr}\left(UB\hat{V}_1B^TU^T\right) - 2n\lambda \\ &= 2\mathrm{Tr}(D) - 2n\lambda \\ &= 2n\left[\frac{1}{n}\sum_{i=1}^{n} d_i - \left(\prod_{i=1}^{n} d_i\right)^{1/n}\right] \end{aligned} \tag{7}$$

But equation (7) is nonnegative, by Lemma 1, with equality holding if and only if $d_1 = d_2 = \cdots = d_n$, in which case $B\hat{V}_1B^T = \lambda I$, which was to be demonstrated. Note that Aw exists if $\hat{V}_1$ is positive definite. Indeed Aw = EV, where E is the matrix whose columns are the eigenvectors of $\hat{V}_1$ and V is a diagonal matrix whose *ith* diagonal element is λ/β_i, i = 1, 2, ···, n, where β_i = *ith* eigenvalue of $\hat{V}_1$.

Theorem 1 associates with each sample W ∈ P, a transformation, A_W, with the property that A_W causes W to cluster in a spherical fashion after transformation with uncorrelated variates having equal variances. If W and Z are samples from populations π_1 and π_2 and if A and B are selected such that

$$A = \lambda_1^{-1/2}A_0 \quad ; \quad B = \lambda_2^{-1/2}B_0 \tag{8}$$

where $\lambda_1 = [\mathrm{Det}(\hat{V}_1)]^{1/n}$, $\lambda_2 = [\mathrm{Det}(\hat{V}_2)]^{1/n}$, and A_0 and B_0 are determined independently for W and Z, respectively, by Theorem 1, the effect is that of a normalization of the intraset similarity in that not only are the intraset distances minimal but $S_A(W,W) = S_B(Z,Z) = 2n$ as well (i.e., the normalization gives each intraset similarity the same value). Moreover, if instead of a threshold of zero in the Sebestyen decision rule [see eq. (5)], we choose the threshold

$$T = \ln \frac{\mathrm{Det}(\hat{V}_1) p_2}{\mathrm{Det}(\hat{V}_2) p_1} \tag{9}$$

the resulting decision rule is the Bayes maximum likelihood decision rule [6] (when the population distributions are Normal) with equal costs of misclassification and *a priori* probabilities p_1 and p_2 for π_1 and π_2, respectively.

4. THE ESTIMATE FOR β

In the weighted least-squares procedure, an estimator of β was selected which minimized $(Y - X\beta)^T V^{-1} (Y - X\beta)$. The optimal estimate is specified in equation (1) and the significance of such an estimator is that of being able to predict, or adjust in some applications, Y to a given matrix X. Since V is ordinarily unknown, we proceed as described below.

Collect N sample values; denote this sample by

$W = \{Y_1, Y_2, \cdots, Y_N\}$ and the sample variance-covariance matrix by

$$\hat{V} = \frac{1}{N} \sum_{i=1}^{N} \left(Y_i - \overline{Y}\right)\left(Y_i - \overline{Y}\right)^T \tag{10}$$

If A is selected such that

$$A\hat{V}A^T = \lambda I \tag{11}$$

where

$$\lambda = [\mathrm{Det}(\hat{V})]^{1/n} \tag{12}$$

then Theorem 1 guarantees that the similarity of W with itself is a minimum after transformation by A. For prediction or adjustment purposes, what we now want to do is to select the vector $Z = X\beta$ which, after transformation, is more similar to the representative sample W than any other such vector. Equivalently, we want to select β such that $S_A(W,\{Z\})$ is a minimum where $Z = X\beta$ and A satisfies equation (11).

Theorem 2: The value of β which minimizes $S_A(W,X\beta)$ is given by

$$\hat{\beta} = \left(X^T\hat{V}^{-1}X\right)^{-1}X^T\hat{V}^{-1}\bar{Y} \tag{13}$$

where $\hat{V}$ is the sample variance-covariance matrix of W, A is the transformation specified in Theorem 1, and $\bar{Y}$ is the sample mean of W.

Proof: From Property 6 of S_A,

$$S_A(W,X\beta) = \mathrm{Tr}(A\hat{V}A^T) + (\bar{Y} - X\beta)^TA^TA(\bar{Y} - X\beta) \tag{14}$$

Differentiating this expression with respect to β, equating to 0, and solving for β yields

$$\hat{\beta} = \left(X^TA^TAX\right)^{-1}X^TA^TA\bar{Y} \tag{15}$$

However, from the condition that $A\hat{V}A^T = \lambda I$

$$A^TA = (1/\lambda)\hat{V}^{-1} \tag{16}$$

which results in equation (8) after substitution into equation (9), which was to be demonstrated.

Under the normality assumption on Y [i.e., $y \sim MVN(X\beta, V)$] where V is unknown, $\hat{V}$ and $\bar{Y}$ are independent; therefore

$$\left.\begin{aligned} E(\hat{\beta}) &= E\left[\left(X^T\hat{V}^{-1}X\right)^{-1}X^T\hat{V}^{-1}\bar{Y}\right] \\ &= E\left[\left(X^T\hat{V}^{-1}X\right)^{-1}X^T\hat{V}^{-1}\right]E(\bar{Y}) \\ &= E\left[\left(X^T\hat{V}^{-1}X\right)^{-1}X^T\hat{V}^{-1}\right]X\beta \\ &= E\left[\left(X^T\hat{V}^{-1}X\right)^{-1}X^T\hat{V}^{-1}X\right]\beta \\ &= \beta \end{aligned}\right\} \qquad (17)$$

Consequently, $\hat{\beta}$ is unbiased under these conditions.

5. SUMMARY

An estimate, $\hat{\beta}$, of β in the linear model $Y = X\beta + \varepsilon$ was obtained such that $X\hat{\beta}$ yielded maximal similarity to the sample $Y_1, Y_2, \cdots, Y_N$ via the Sebestyen similarity function. The unobservable random error term, ε, was assumed to satisfy $E(\varepsilon) = 0$ (the zero vector) and $E(\varepsilon\varepsilon^T) = V$, with V assumed to be unknown. The resulting estimate is seen to be in the same form as the standard Gauss-Markov estimate

$$\hat{\beta} = \left(X^TV^{-1}X\right)^{-1}X^TV^{-1}Y \qquad (18)$$

except V is replaced by the standard (and under the normality assumption, the maximum likelihood) estimate of the variance-covariance matrix.

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